



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 06:22 PM GMT

PDB ID : 4KBV
Title : 70S ribosome translocation intermediate GDPNP-II containing elongation factor EFG/GDPNP, mRNA, and tRNA bound in the pe*/E state. This entry contains 30S ribosomal subunit B. The full asymmetric unit also contains PDB entries 4KBW (50S subunit B), 4KBT (30S subunit A), and 4KBU (50S subunit A).
Authors : Zhou, J.; Lancaster, L.; Donohue, J.P.; Noller, H.F.
Deposited on : 2013-04-23
Resolution : 3.86 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

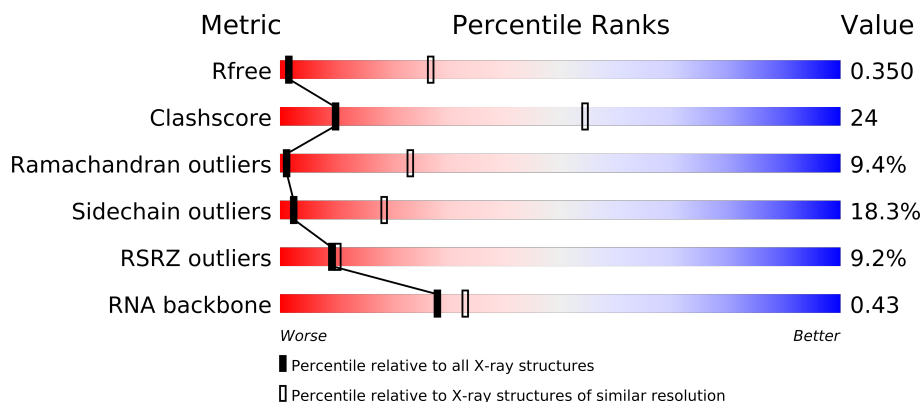
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.86 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1013 (4.30-3.42)
Clashscore	79885	1145 (4.22-3.50)
Ramachandran outliers	78287	1091 (4.22-3.50)
Sidechain outliers	78261	1081 (4.22-3.50)
RSRZ outliers	66119	1014 (4.30-3.42)
RNA backbone	1838	1010 (4.84-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	B	235	
2	C	207	
3	D	208	
4	E	151	
5	F	101	
6	G	155	
7	H	138	
8	I	127	
9	J	99	
10	K	119	
11	L	125	
12	M	125	

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Mol	Chain	Length	Quality of chain
13	N	60	
14	O	88	
15	P	84	
16	Q	100	
17	R	70	
18	S	79	
19	T	99	
20	A	1511	
21	V	18	
22	W	77	
23	Y	687	
24	U	6	

2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 58977 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	235	Total	C	N	O	S	0	0	0
			1910	1218	342	345	5			

- Molecule 2 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	207	Total	C	N	O	S	0	0	0
			1621	1022	315	283	1			

- Molecule 3 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 4 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	151	Total	C	N	O	S	0	0	0
			1156	729	218	205	4			

- Molecule 5 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 6 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 7 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 8 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	127	Total	C	N	O	S	0	0	0
			1011	639	198	174				

- Molecule 9 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	99	Total	C	N	O	S	0	0	0
			802	504	157	140	1			

- Molecule 10 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	K	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

- Molecule 11 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	125	Total	C	N	O	S	0	0	0
			976	614	196	165	1			

- Molecule 12 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	125	Total	C	N	O	S	0	0	0
			997	617	207	171	2			

- Molecule 13 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 14 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	O	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 15 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	P	84	Total	C	N	O	S	0	0	0
			706	446	140	119	1			

- Molecule 16 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	Q	100	Total	C	N	O	S	0	0	0
			835	534	156	143	2			

- Molecule 17 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	R	70	Total	C	N	O	S	0	0	0
			574	367	112	95				

- Molecule 18 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	S	79	Total	C	N	O	S	0	0	0
			634	405	115	112	2			

- Molecule 19 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	T	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			

- Molecule 20 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	A	1511	Total	C	N	O	P	0	0	0
			32474	14455	6015	10494	1510			

- Molecule 21 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	V	18	Total	C	N	O	P	0	0	0
			393	177	81	118	17			

- Molecule 22 is a RNA chain called tRNA-Met.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	W	77	Total	C	N	O	P	0	0	0
			1635	732	291	536	76			

- Molecule 23 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	Y	687	Total	C	N	O	S	0	0	0
			5380	3414	922	1024	20			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	129	LYS	HIS	CONFLICT	UNP Q72I01
Y	226	ASN	HIS	CONFLICT	UNP Q72I01

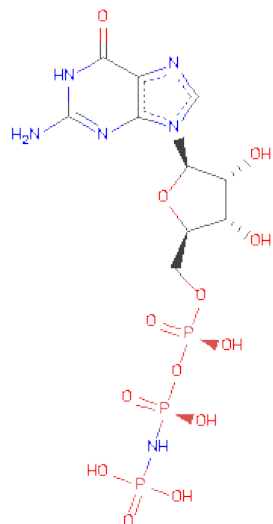
- Molecule 24 is a protein called Viomycin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
24	U	6	Total	C	N	O	0	0	0
			48	25	13	10			

- Molecule 25 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	Y	1	Total	Mg	0	0
			1	1		

- Molecule 26 is PHOSPHOAMINOPHOSPHONICACID-GUANYLATE ESTER (three-letter code: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃).



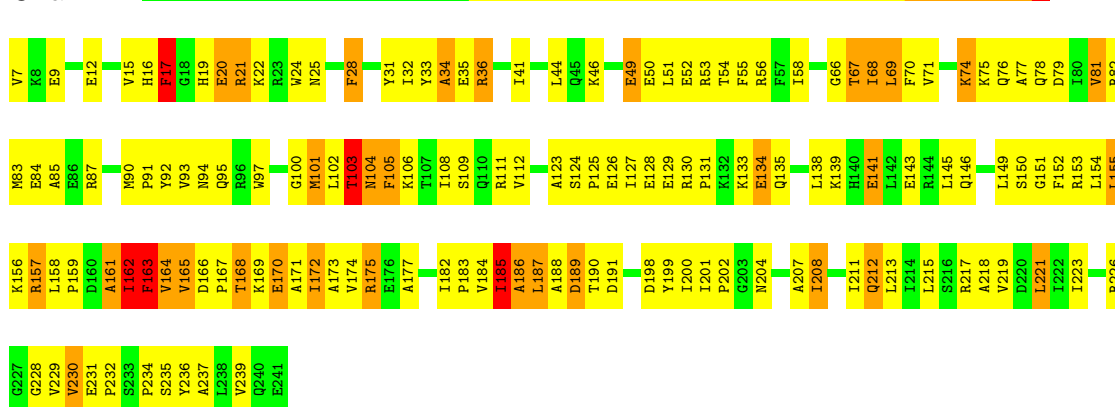
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
26	Y	1	32	10	6	13	3	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

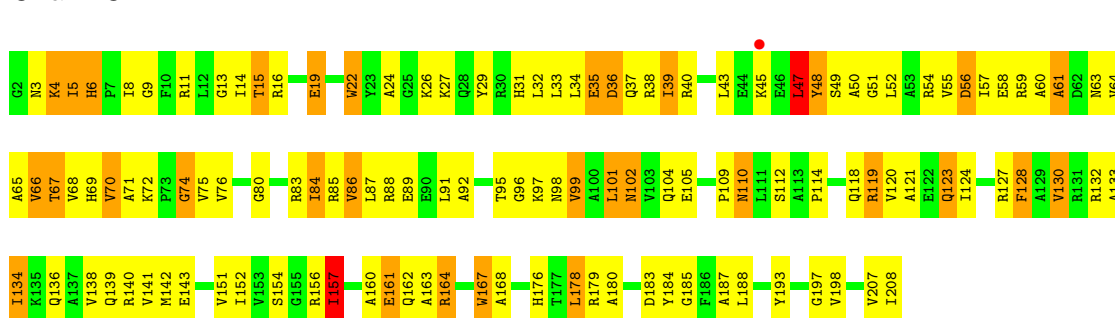
• Molecule 1: 30S ribosomal protein S2

Chain B:



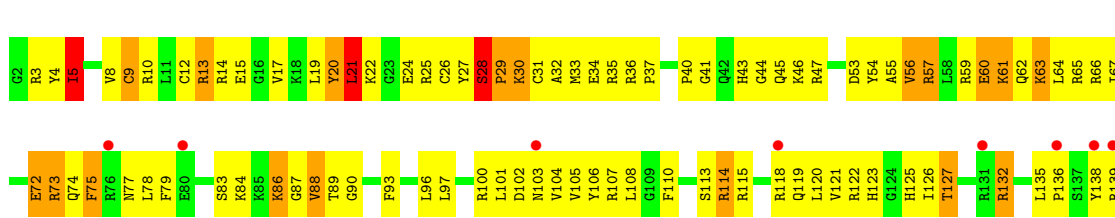
• Molecule 2: 30S ribosomal protein S3

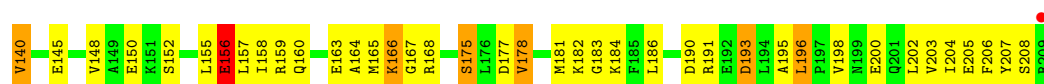
Chain C:



• Molecule 3: 30S ribosomal protein S4

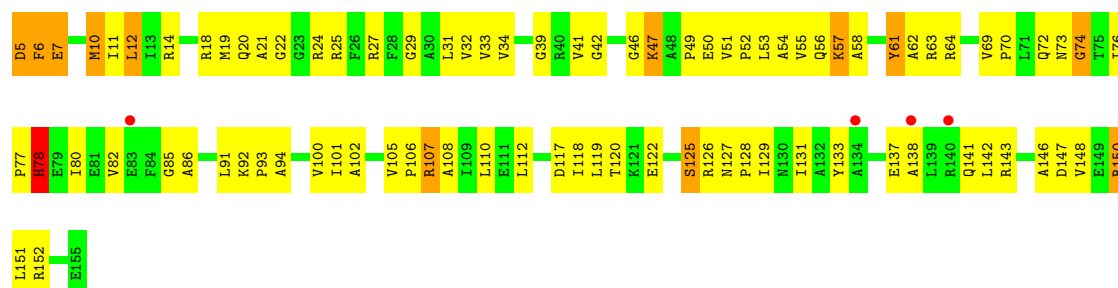
Chain D:





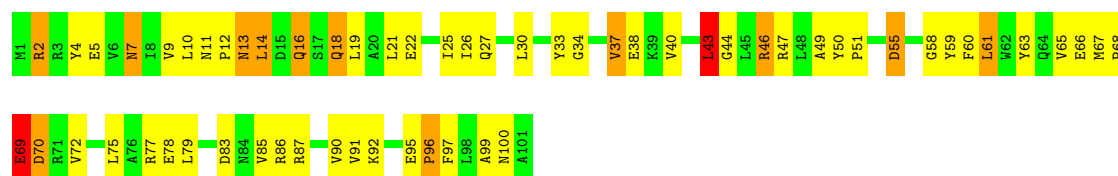
• Molecule 4: 30S ribosomal protein S5

Chain E:



• Molecule 5: 30S ribosomal protein S6

Chain F:



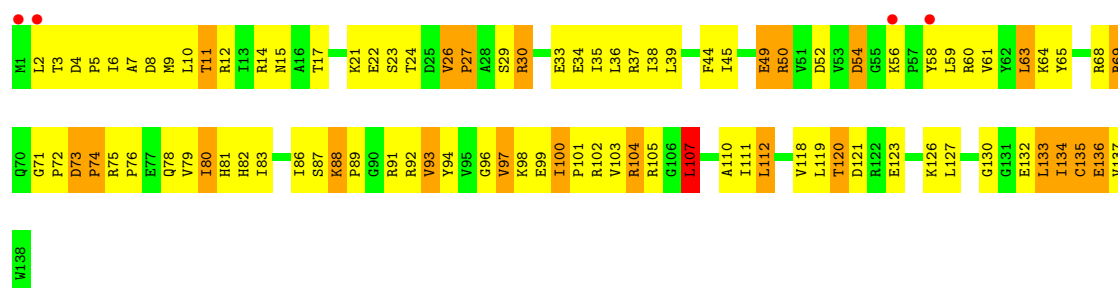
• Molecule 6: 30S ribosomal protein S7

Chain G:



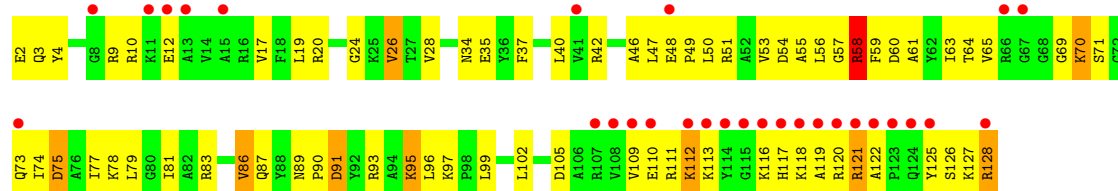
• Molecule 7: 30S ribosomal protein S8

Chain H:



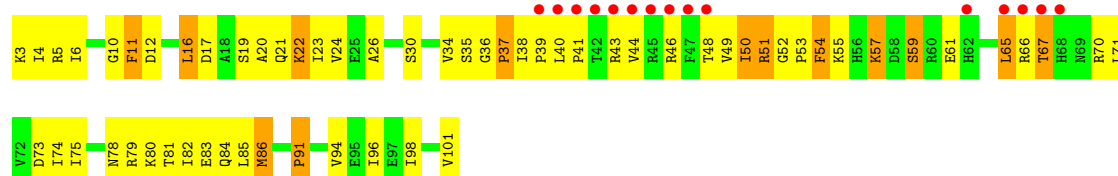
• Molecule 8: 30S ribosomal protein S9

Chain I: 



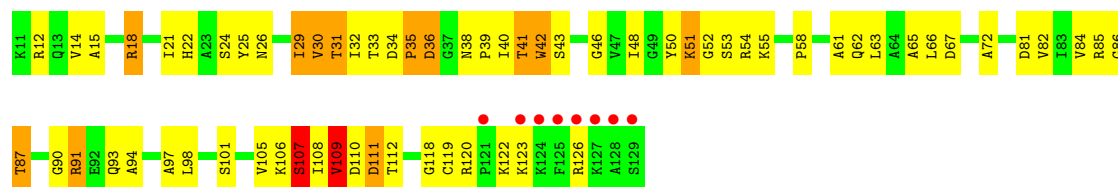
- Molecule 9: 30S ribosomal protein S10

Chain J: 



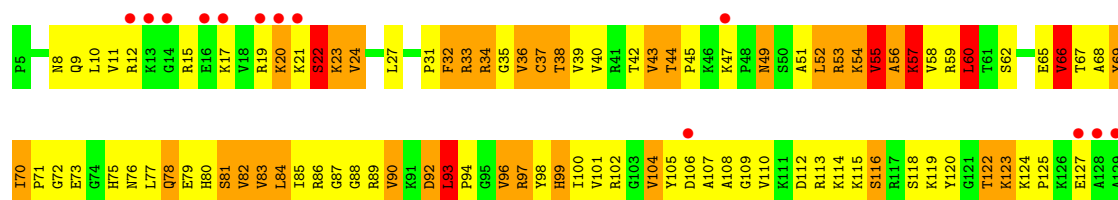
- Molecule 10: 30S ribosomal protein S11

Chain K: 



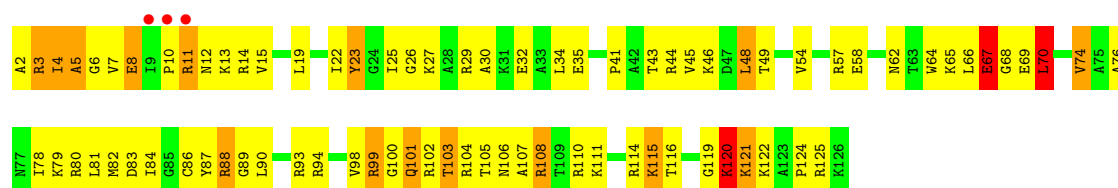
- Molecule 11: 30S ribosomal protein S12

Chain L: 



- Molecule 12: 30S ribosomal protein S13

Chain M: 



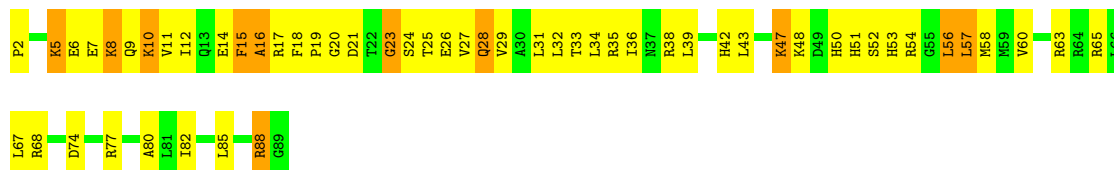
- Molecule 13: 30S ribosomal protein S14 type Z

Chain N: 



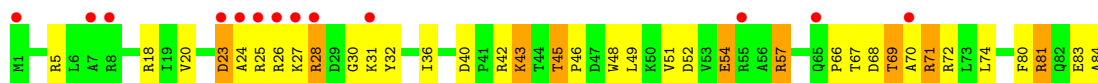
• Molecule 14: 30S ribosomal protein S15

Chain O:



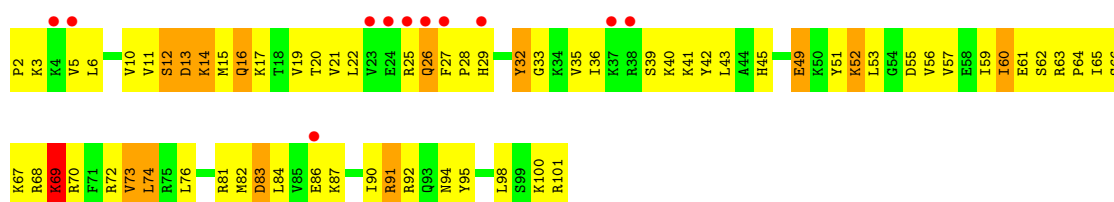
• Molecule 15: 30S ribosomal protein S16

Chain P:



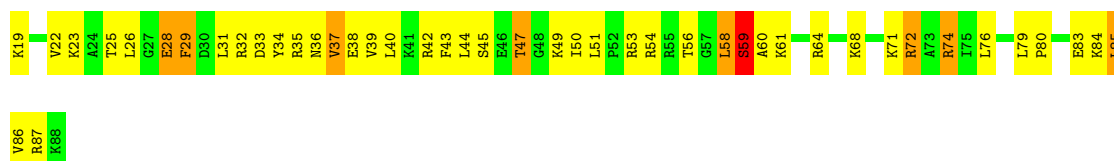
• Molecule 16: 30S ribosomal protein S17

Chain Q:



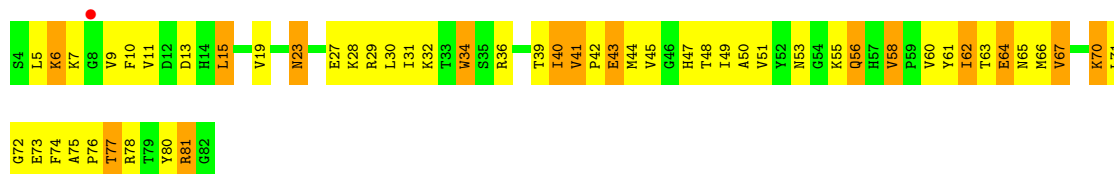
• Molecule 17: 30S ribosomal protein S18

Chain R:



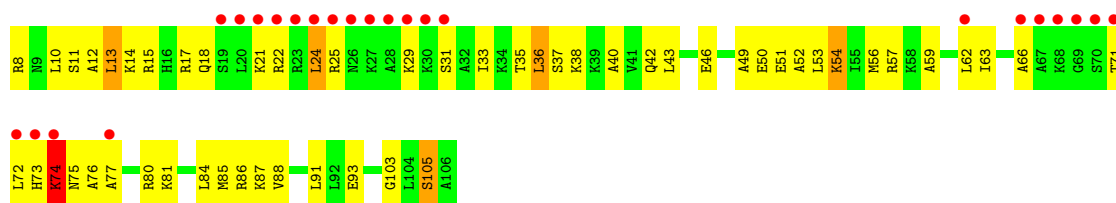
• Molecule 18: 30S ribosomal protein S19

Chain S:



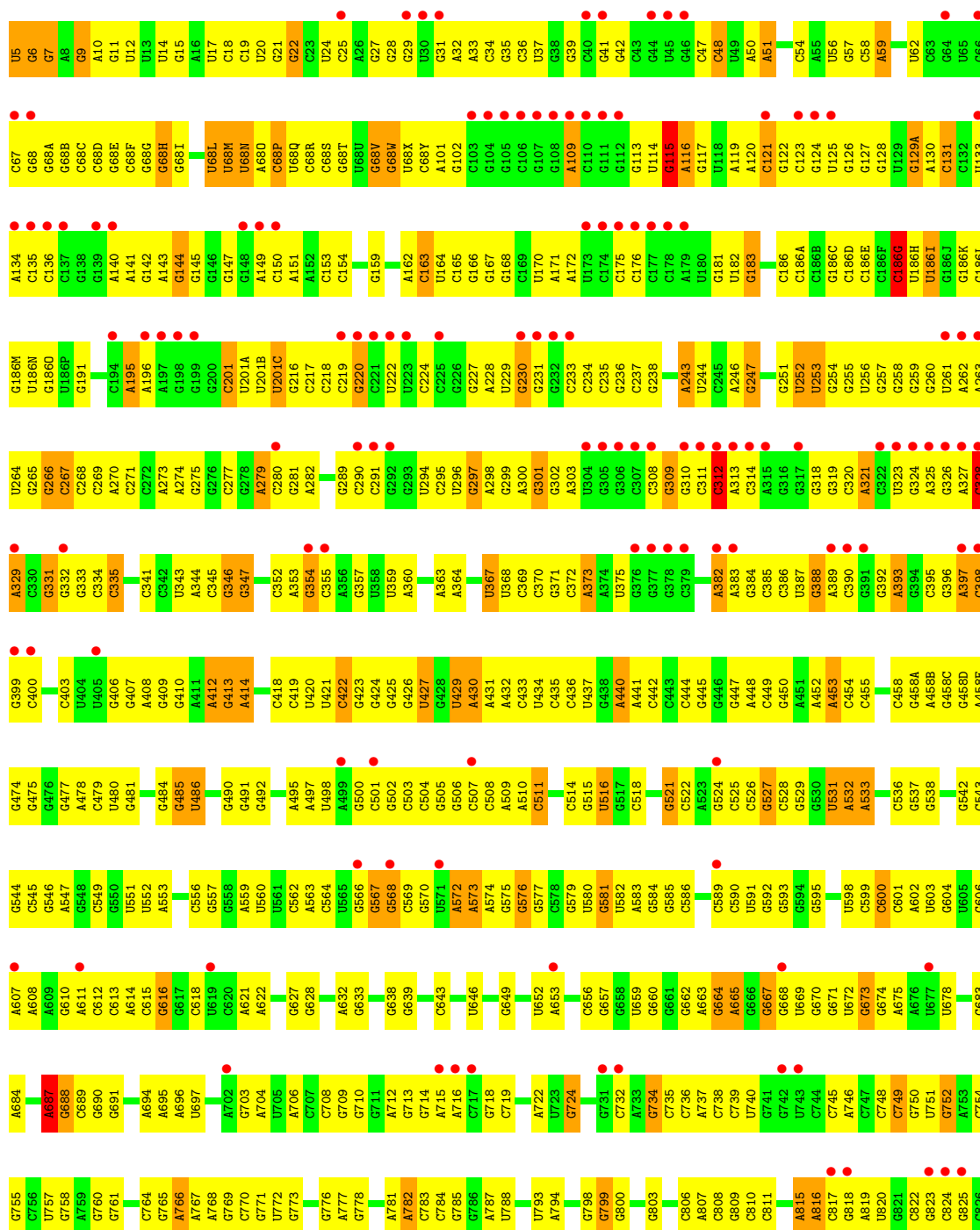
• Molecule 19: 30S ribosomal protein S20

Chain T:

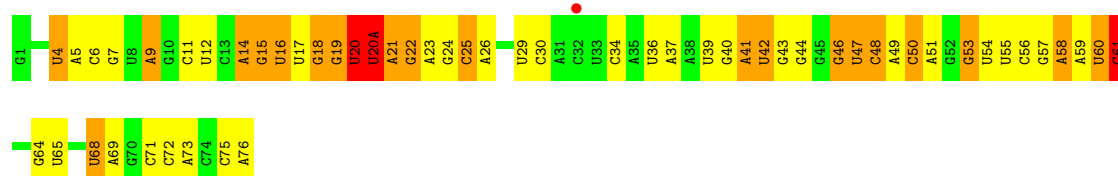


• Molecule 20: 16S ribosomal RNA

Chain A:

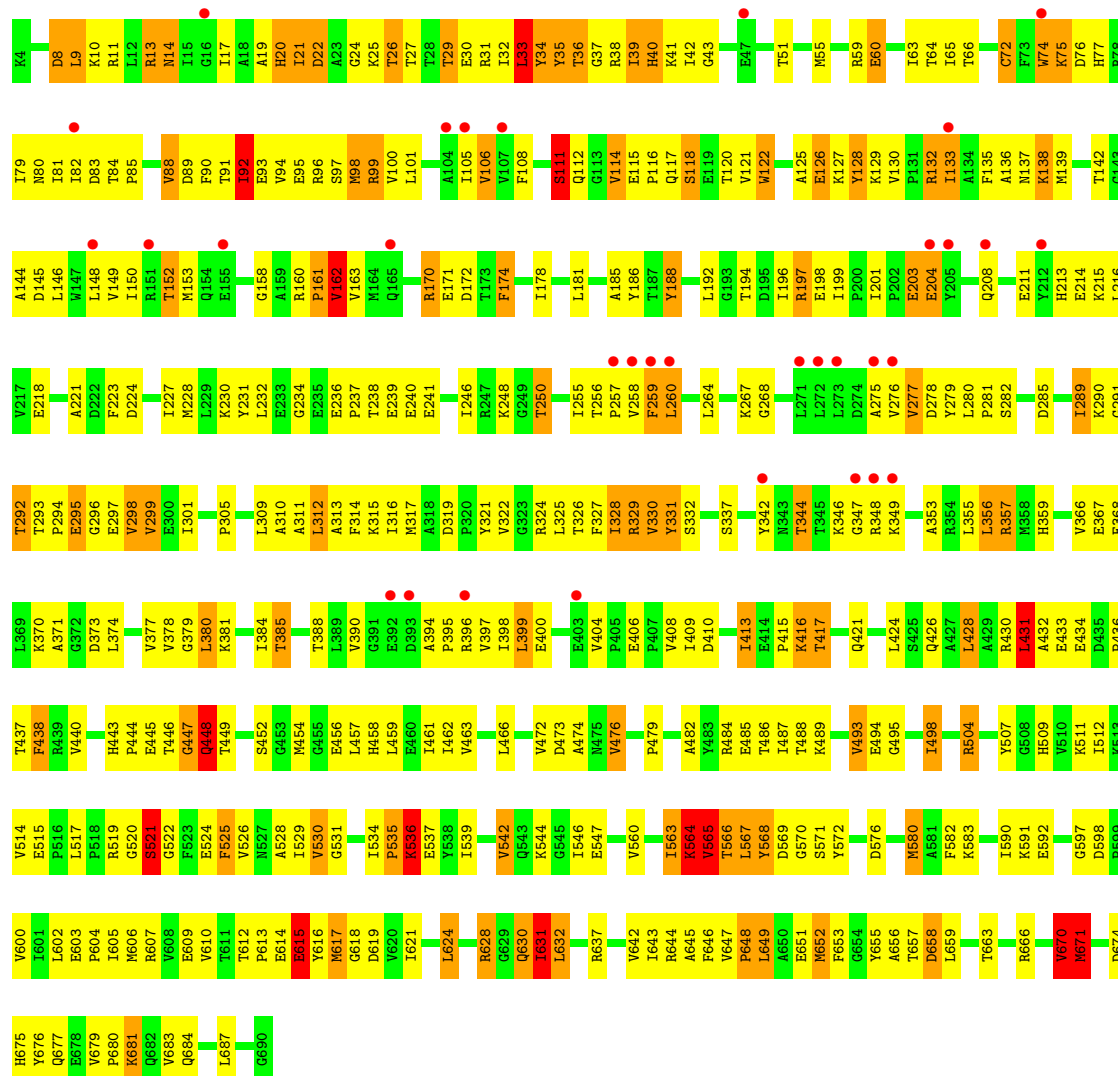






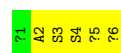
• Molecule 23: Elongation factor G

Chain Y:



• Molecule 24: Viomycin

Chain U:



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	302.39Å 683.92Å 356.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.86 182.04 – 3.87	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.86) 64.4 (182.04-3.87)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.34	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 3.89Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.264 , 0.317 0.351 , 0.350	Depositor DCC
R_{free} test set	21649 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	76.3	Xtriage
Anisotropy	0.322	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 289.2	EDS
Estimated twinning fraction	0.320 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.24$, $\langle L^2 \rangle = 0.09$	Xtriage
Outliers	0 of 432130 reflections	Xtriage
F_o, F_c correlation	0.54	EDS
Total number of atoms	58977	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GNP, DPP, MG, KBE, UAL, 5OH

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	B	0.43	0/1945	0.80	6/2621 (0.2%)
2	C	0.30	0/1645	0.58	0/2216
3	D	0.30	0/1733	0.59	0/2318
4	E	0.30	0/1172	0.58	0/1576
5	F	0.28	0/856	0.56	0/1154
6	G	0.29	0/1276	0.53	0/1709
7	H	0.31	0/1136	0.61	0/1527
8	I	0.32	0/1029	0.56	1/1378 (0.1%)
9	J	0.30	0/815	0.55	0/1095
10	K	0.39	0/900	0.67	0/1213
11	L	0.47	0/992	0.88	2/1327 (0.2%)
12	M	0.27	0/1008	0.59	0/1347
13	N	0.30	0/501	0.49	0/664
14	O	0.32	0/745	0.62	0/992
15	P	0.27	0/722	0.52	0/970
16	Q	0.41	0/848	0.73	0/1131
17	R	0.29	0/579	0.61	0/768
18	S	0.30	0/647	0.61	0/870
19	T	0.33	0/764	0.61	0/1006
20	A	0.38	2/36351 (0.0%)	1.06	96/56736 (0.2%)
21	V	0.29	0/443	0.86	0/691
22	W	0.37	0/1827	1.06	7/2845 (0.2%)
23	Y	0.41	0/5481	0.69	3/7418 (0.0%)
24	U	1.09	0/11	1.84	0/13
All	All	0.37	2/63426 (0.0%)	0.93	115/93585 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	3
11	L	0	2
23	Y	0	4
All	All	0	9

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	1393	U	N1-C2	9.25	1.46	1.38
20	A	1393	U	C2-O2	5.28	1.27	1.22

The worst 5 of 115 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	1393	U	N1-C2-O2	12.43	131.50	122.80
20	A	815	A	C5-C6-N6	11.09	132.57	123.70
20	A	815	A	N1-C6-N6	-10.71	112.17	118.60
20	A	1393	U	N3-C4-C5	10.67	121.00	114.60
23	Y	33	LEU	CA-CB-CG	9.39	136.91	115.30

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	170	GLU	Peptide
1	B	185	ILE	Peptide
1	B	68	ILE	Peptide
11	L	32	PHE	Peptide
11	L	57	LYS	Peptide

5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1910	0	1957	120	0
2	C	1621	0	1688	86	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	1703	0	1763	116	0
4	E	1156	0	1213	62	0
5	F	843	0	857	46	0
6	G	1257	0	1296	82	0
7	H	1116	0	1177	83	0
8	I	1011	0	1043	58	0
9	J	802	0	849	59	0
10	K	885	0	904	54	0
11	L	976	0	1062	108	0
12	M	997	0	1072	67	0
13	N	492	0	529	24	0
14	O	734	0	771	40	0
15	P	706	0	725	29	0
16	Q	835	0	906	71	0
17	R	574	0	644	42	0
18	S	634	0	655	41	0
19	T	762	0	859	44	0
20	A	32474	0	16393	1045	0
21	V	393	0	197	14	0
22	W	1635	0	831	66	0
23	Y	5380	0	5436	307	0
24	U	48	0	41	15	0
25	Y	1	0	0	0	0
26	Y	32	0	13	18	0
All	All	58977	0	42881	2409	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 24.

The worst 5 of 2409 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
22:W:50:C:N4	22:W:64:G:H1	1.36	1.22
23:Y:30:GLU:O	23:Y:33:LEU:N	1.79	1.13
20:A:369:C:N4	20:A:392:G:H1	1.46	1.11
20:A:1007:C:N4	20:A:1022:G:H1	1.47	1.10
20:A:815:A:C2	20:A:1527:C:O2	2.03	1.10

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	233/235 (99%)	164 (70%)	49 (21%)	20 (9%)	1	26
2	C	205/207 (99%)	136 (66%)	47 (23%)	22 (11%)	1	17
3	D	206/208 (99%)	140 (68%)	49 (24%)	17 (8%)	1	27
4	E	149/151 (99%)	125 (84%)	16 (11%)	8 (5%)	3	41
5	F	99/101 (98%)	81 (82%)	10 (10%)	8 (8%)	1	28
6	G	153/155 (99%)	116 (76%)	24 (16%)	13 (8%)	1	26
7	H	136/138 (99%)	90 (66%)	29 (21%)	17 (12%)	1	14
8	I	125/127 (98%)	100 (80%)	16 (13%)	9 (7%)	2	32
9	J	97/99 (98%)	71 (73%)	20 (21%)	6 (6%)	2	37
10	K	117/119 (98%)	82 (70%)	22 (19%)	13 (11%)	1	17
11	L	123/125 (98%)	54 (44%)	41 (33%)	28 (23%)	0	2
12	M	123/125 (98%)	85 (69%)	22 (18%)	16 (13%)	0	13
13	N	58/60 (97%)	45 (78%)	8 (14%)	5 (9%)	1	26
14	O	86/88 (98%)	60 (70%)	20 (23%)	6 (7%)	2	33
15	P	82/84 (98%)	59 (72%)	20 (24%)	3 (4%)	5	53
16	Q	98/100 (98%)	72 (74%)	17 (17%)	9 (9%)	1	24
17	R	68/70 (97%)	49 (72%)	16 (24%)	3 (4%)	4	47
18	S	77/79 (98%)	38 (49%)	29 (38%)	10 (13%)	0	13
19	T	97/99 (98%)	79 (81%)	14 (14%)	4 (4%)	4	49
23	Y	685/687 (100%)	476 (70%)	143 (21%)	66 (10%)	1	22
24	U	2/6 (33%)	2 (100%)	0	0	100	100
All	All	3019/3063 (99%)	2124 (70%)	612 (20%)	283 (9%)	1	23

5 of 283 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	20	GLU

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Mol	Chain	Res	Type
1	B	34	ALA
1	B	67	THR
1	B	76	GLN
1	B	103	THR

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	203/203 (100%)	165 (81%)	38 (19%)	2	18
2	C	161/161 (100%)	121 (75%)	40 (25%)	1	8
3	D	180/180 (100%)	149 (83%)	31 (17%)	3	22
4	E	116/116 (100%)	93 (80%)	23 (20%)	2	15
5	F	90/90 (100%)	74 (82%)	16 (18%)	2	20
6	G	126/126 (100%)	106 (84%)	20 (16%)	4	28
7	H	119/119 (100%)	99 (83%)	20 (17%)	3	24
8	I	98/98 (100%)	82 (84%)	16 (16%)	3	26
9	J	89/89 (100%)	74 (83%)	15 (17%)	3	24
10	K	90/90 (100%)	78 (87%)	12 (13%)	6	37
11	L	104/104 (100%)	77 (74%)	27 (26%)	1	7
12	M	100/100 (100%)	82 (82%)	18 (18%)	2	19
13	N	49/49 (100%)	40 (82%)	9 (18%)	2	18
14	O	79/79 (100%)	62 (78%)	17 (22%)	1	11
15	P	72/72 (100%)	60 (83%)	12 (17%)	3	25
16	Q	95/95 (100%)	82 (86%)	13 (14%)	5	35
17	R	61/61 (100%)	48 (79%)	13 (21%)	1	12
18	S	69/69 (100%)	54 (78%)	15 (22%)	1	11
19	T	76/76 (100%)	69 (91%)	7 (9%)	13	56
23	Y	579/579 (100%)	472 (82%)	107 (18%)	2	18
24	U	2/2 (100%)	2 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2558/2558 (100%)	2089 (82%)	469 (18%)	2 18

5 of 469 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	J	65	LEU
12	M	43	THR
23	Y	424	LEU
9	J	96	ILE
11	L	52	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
7	H	78	GLN
9	J	84	GLN
23	Y	448	GLN
8	I	124	GLN
9	J	76	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
20	A	1511/1511 (100%)	304 (20%)	18 (1%)
21	V	17/18 (94%)	8 (47%)	1 (5%)
22	W	76/77 (98%)	22 (28%)	2 (2%)
All	All	1604/1606 (99%)	334 (20%)	21 (1%)

5 of 334 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
20	A	6	G
20	A	7	G
20	A	9	G
20	A	22	G
20	A	29	G

5 of 21 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
20	A	748	C
20	A	1064	G
20	A	1537	U
20	A	687	A
21	V	8	A

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
24	KBE	U	1	24	8,8,9	8.66	1 (12%)	6,8,10	1.01	1 (16%)
24	DPP	U	2	24	5,5,6	6.98	1 (20%)	3,5,7	2.65	2 (66%)
24	UAL	U	5	24	7,8,9	1.43	1 (14%)	6,9,11	1.03	0
24	5OH	U	6	24	12,12,13	6.58	3 (25%)	13,16,18	0.85	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	KBE	U	1	24	-	0/6/7/8	0/0/0/0
24	DPP	U	2	24	-	0/2/4/6	0/0/0/0
24	UAL	U	5	24	-	0/3/7/9	0/0/0/0
24	5OH	U	6	24	-	0/2/18/20	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	U	1	KBE	O-C	24.35	1.28	1.11
24	U	6	5OH	O-C	22.02	1.26	1.11
24	U	2	DPP	O-C	15.38	1.22	1.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	U	6	5OH	CQ-NP	5.08	1.40	1.34
24	U	6	5OH	CQ-NR	2.40	1.40	1.32

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	U	2	DPP	C-CA-N	3.85	117.68	113.83
24	U	2	DPP	CB-CA-N	-2.48	103.17	111.50
24	U	1	KBE	CG-CB-CA	2.13	115.07	111.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
26	GNP	Y	702	25	34,34,34	1.72	6 (17%)	50,54,54	5.62	14 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	GNP	Y	702	25	-	0/18/38/38	0/1/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	Y	702	GNP	PG-O1G	6.13	1.53	1.46
26	Y	702	GNP	PB-N3B	-4.52	1.60	1.64
26	Y	702	GNP	PA-O3A	-2.67	1.55	1.59
26	Y	702	GNP	PB-O3A	-2.30	1.55	1.59
26	Y	702	GNP	PA-O2A	-2.15	1.45	1.55

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	Y	702	GNP	C6-C5-N7	-37.55	129.08	134.14
26	Y	702	GNP	PA-O3A-PB	-4.60	116.10	131.81
26	Y	702	GNP	C2-N3-C4	-3.75	109.82	115.09
26	Y	702	GNP	C4'-O4'-C1'	-3.69	105.75	109.75
26	Y	702	GNP	C4-C5-N7	3.50	112.52	109.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	B	235/235 (100%)	-0.38	0 100 100	26, 78, 150, 182	0
2	C	207/207 (100%)	-0.15	1 (0%) 88 76	33, 66, 122, 164	0
3	D	208/208 (100%)	0.29	9 (4%) 34 26	16, 79, 141, 186	0
4	E	151/151 (100%)	-0.07	4 (2%) 53 39	23, 71, 126, 185	0
5	F	101/101 (100%)	-0.37	0 100 100	29, 64, 127, 176	0
6	G	155/155 (100%)	-0.10	3 (1%) 64 47	39, 86, 144, 209	0
7	H	138/138 (100%)	-0.15	4 (2%) 49 36	33, 67, 126, 179	0
8	I	127/127 (100%)	1.03	29 (22%) 1 2	16, 69, 128, 177	0
9	J	99/99 (100%)	0.55	15 (15%) 3 4	24, 81, 132, 167	0
10	K	119/119 (100%)	0.01	8 (6%) 17 16	37, 83, 128, 165	0
11	L	125/125 (100%)	0.26	13 (10%) 7 9	21, 72, 139, 179	0
12	M	125/125 (100%)	-0.24	3 (2%) 56 41	58, 97, 159, 195	0
13	N	60/60 (100%)	1.90	26 (43%) 1 1	30, 54, 113, 147	0
14	O	88/88 (100%)	-0.27	0 100 100	32, 73, 127, 165	0
15	P	84/84 (100%)	0.76	13 (15%) 3 4	29, 73, 132, 175	0
16	Q	100/100 (100%)	0.37	11 (11%) 6 8	42, 74, 130, 159	0
17	R	70/70 (100%)	-0.18	0 100 100	26, 69, 132, 198	0
18	S	79/79 (100%)	-0.11	1 (1%) 74 57	26, 89, 165, 199	0
19	T	99/99 (100%)	1.03	24 (24%) 1 2	27, 80, 144, 169	0
20	A	1511/1511 (100%)	0.67	224 (14%) 3 4	6, 84, 166, 265	0
21	V	18/18 (100%)	1.62	6 (33%) 1 2	33, 135, 179, 181	0
22	W	77/77 (100%)	-0.21	1 (1%) 74 57	43, 116, 183, 208	0
23	Y	687/687 (100%)	0.01	33 (4%) 29 23	25, 86, 158, 217	0
24	U	2/6 (33%)	-0.25	0 100 100	66, 66, 66, 66	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	4665/4669 (99%)	0.29	428 (9%) 9 10	6, 81, 156, 265	0

The worst 5 of 428 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
20	A	134	A	17.1
20	A	135	C	13.0
20	A	325	A	11.4
20	A	328	C	10.4
8	I	124	GLN	9.5

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
24	DPP	U	2	6/7	0.15	-	65,65,65,65	0
24	UAL	U	5	9/10	0.13	-	65,65,65,65	0
24	KBE	U	1	9/10	0.17	-	65,65,65,65	0
24	5OH	U	6	12/13	0.32	-	99,101,102,102	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
25	MG	Y	701	1/1	0.14	-	104,104,104,104	0
26	GNP	Y	702	32/32	0.23	-	58,71,81,83	0

6.5 Other polymers

There are no such residues in this entry.